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Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources

Quarterly Progress Report (April – June 2014)

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EXECUTIVE SUMMARY

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program, part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah, is focused on engineering, scientific, and legal research surrounding the development of these resources in Utah.

Outreach efforts in Task 2 have continued to focus on disseminating results from the various subtasks and on fielding interview requests. Two papers from this program have been submitted for presentation at the 35th Oil Shale Symposium in Golden, CO, in October 2014.

Task 3 focuses on utilization of oil shale and oil sands resources with CO₂ management. The Subtask 3.1 team focused on organizing and interpreting emission factors associated with natural gas production and processing. The Subtask 3.3 and 3.4 teams completed a skeletal model (composed of component modules) for conventional oil and gas development in the Uinta Basin, including a module for estimating CO₂ equivalent (CO2e) emissions that uses data provided by Subtask 3.1.

Task 4 projects are related to liquid fuel production by in-situ thermal processing of oil shale. Subtask 4.1 researchers have added a flow through porous media simulation strategy to their suite of simulation tools for modeling oil production from a bed of rubberized oil shale. The Subtask 4.3 team has been working on a mechanistic model of oil shale kerogen pyrolysis based on the Chemical Percolation Devolatilization model. In the model, light gases are assumed to come from char bridge formation and heavy gases from aliphatic bridge cleavage. These assumptions result in good agreement with the kerogen retort data for the three kerogen samples studied.

Task 5 and 6 projects relate to environmental, legal, economic, and policy analysis. A final topical report on policy and economic issues associated with using simulation to assess environmental impacts (Subtask 5.3) has not been submitted. All Task 6 projects are now complete.

Task 7 researchers are completing research projects with their industrial partner, American Shale Oil (AMSO). The Subtask 7.1 team has been developing reservoir scale simulations using FLAC3D to simulate the entire reservoir development process, including heating, porosity and permeability development, and associated stress and deformation changes. They are also using the software to simulate their triaxial testing data. Subtask 7.3 researchers completed simulations of AMSO heater tests and reported their results to AMSO. They also began simulations using a much larger domain (e.g. five wells) that better represents a commercial-scale in-situ production operation.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

There were no schedule/cost variances or other situations requiring updating/amending of the Project Management Plan (PMP) in this quarter.

Task 2.0 -Technology Transfer and Outreach

Technology transfer and outreach efforts are focused on communicating project results through publication of papers and reports, through visits and interviews, and through updates of the program website. In this quarter, one paper was published (Subtask 4.9), Dr. Jennifer Spinti spoke to a reporter for the Grand Junction Daily Sentinel and was quoted in a subsequent article, and researchers from all subtasks within the program agreed to submit an oil shale book outline to a publisher for possible publication in book form of research resulting from this program.

Task 3.0 - Clean Oil Shale and Oil Sands Utilization with CO₂ Management

<u>Subtask 3.1 – Lifecycle Greenhouse Gas Analysis of Conventional Oil and Gas Development in</u> <u>the Uinta Basin (PI: Kerry Kelly, David Pershing)</u>

During this quarter, the team focused on organizing and interpreting the information about emission factors associated with natural gas production and processing. This information is being compiled into a report, which can be used as part of the oil and gas production module in Subtask 3.3 to estimate greenhouse gas (GHG) emissions associated with oil and gas drilling operations in the Uinta Basin.

The team is also identifying the most appropriate emission factors for the Uinta Basin. GHG emissions associated with oil and gas production occur during site preparation, drilling/ completion, production, processing and transport phases. They take the form of methane as well as combustion (CO_2 , CH_4 , and N_2O) emissions. The extent of methane emissions depends on a variety of factors including: (1) formation properties, (2) the type of process and operating procedures, and (3) the nature and condition of equipment employed. In general, well completion activities (including hydraulic fracturing) tend to dominate potential emissions associated with oil and gas production.

The following tables summarize the range of GHG emission factors available from industry, government agencies and peer-reviewed publications. The emission factors used two types of scaling factors, well counts and gas production. To present the emission factors on a consistent basis, some conversions were made. These published emission estimates vary widely depending on actual differences in emissions (i.e., formation properties, operating procedures, equipment employed), study methods employed (i.e., surveys, measurements collected for individual pieces of equipment, regional measurements of methane and other light hydrocarbon gases), as well as underlying assumptions.

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Activity	Conventional & unconventional	Units CO ₂ e
Production	1.69E-5 - 8.13E-5 *	Metric tons/bbls
Transport	1.81E-8 - 8.38E-8 **	Metric tons/bbls oil transported
* * *		

* ranging from conventional to heavy oil

** ranging from transported by pipeline to transported by tanker truck

 Table 2. Emission factors for gas processing.

÷	Natural	Gas

Activity	Conventional	Unconventional	Units CO ₂ e			
well completion and	(12-15)	1041 0000 *	Metric tons/ billion cubic feet of			
workover		1841-2038 *	natural gas production			
	(12-36)	483-2058	Metric tons/ well			
		2971-6933 **	Metric tons/ well**			
	1481-2922		Metric tons/ billion cubic feet of			
Production		1897-7200	natural gas production			
	1.42-2.75	2.01-7.9	Expressed as % of total production			
	600		Metric tons/ billion cubic feet of			
Processing		1994	natural gas production			
	1108		Metric tons/ billion cubic feet of			
Transmission	1100	1108	natural gas production			
Distribution	665	665				
Transport		34-431	Metric tons/ well			
* estimated as 10% of	all gas vented					

** entire volume of gas release during flowback

Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO₂ Capture (PI: Jennifer Spinti)

Work on this subtask has been limited this year due as the PI is the only project team member remaining. Fortunately, a new graduate student, Oscar Diaz-Ibarra, has joined the team to help wrap up the project. As mentioned in previous quarterly reports, the complex burner geometry of the TEA-C burner, used in the IFRF oxy-combustion tests (Coraggio and Laiola, 2009), has been simulated using Star-CCM+. The velocity magnitude field from this simulation is shown in Figures 1 and 2. The data at the burner exit plane will be filtered to match the mesh resolution of the Arches simulation, which is computed on a much coarser grid, and then used as the Arches inlet boundary condition.



Figure 1. Results of Star-CCM+ simulation of flow through TEA-C burner. Cutaway plane on centerline in flow direction shows velocity magnitude.



Figure 2. Results of Star-CCM+ simulation of flow through TEA-C burner. Cutaway plane at burner exit plane shows velocity field that will be inlet boundary condition to Arches simulation.

Subtask 3.3 - Development of Oil and Gas Production Modules for CLEAR_{uff} (PI: Terry Ring)

Research in this quarter for Subtasks 3.3 and 3.4 has focused on the creation of a skeletal model for conventional oil and gas development in the Uinta Basin, a milestone that is now complete. The purpose of this model is to demonstrate the full functionality of each of the component modules, namely:

- Number of wells drilled per time step over the time period of interest (i.e. drilling schedule)
- Attributes of each well in the drilling schedule, including well type (oil or gas), location (i.e. the oil or gas field the well is located in), decline curve coefficients, well depth, and surface land ownership (federal, state, Indian, or private)
- Amount of oil or gas produced
- Fiscal impacts from conventional oil and gas production (royalties, severance taxes, property taxes, and state and federal corporate income taxes)
- Number of jobs generated
- · Quantity of air pollutants and GHGs emitted
- Water and energy balances

All of these factors are calculated and tracked for each well and, where applicable, for each time step of the model. Uncertainty in the input parameters has been accounted for using Monte-Carlo methods to randomly determine the value for nearly all model input parameters (decline curve coefficients, well depth, GHG emission factors, etc.) based on the probability distributions of values for each of these parameters. By sampling from the probability distributions for each model input parameter for each well in each iteration and then performing the simulation many times, the range of uncertainty in the model outputs is computed.

Examples plots after 20 Monte-Carlo iterations are shown in Figures 3 and 4 for two of the modules. In a single Monte-Carlo iteration, decline curve coefficients are randomly selected for

each of the 7,846 wells drilled during the modeled time period. The resulting production and CO_2 equivalent (CO_2e) emissions from all wells is then calculated.



Total Oil Production - Simulated vs. Actual

Figure 3. Range of simulated oil production volumes versus actual oil production in the Uinta Basin over the 1999 - 2012 time period. Results are generated from actual drilling schedule.



Total CO2 Equivalent Emissions Estimate

Figure 4. Range of CO₂e emissions from oil and gas development, including drilling, completion, hydraulic fracturing, production, separation, processing, transmission and storage. Results are generated from actual drilling schedule and simulated production volumes.

With work on the skeletal model for conventional oil and gas development largely finished, team members will next focus on (1) refining the modules that have the largest impact on the uncertainty of model results (most notably the drilling schedule module) and (2) updating their previous work on modeling unconventional oil development (oil shale and oil sands) to use the same framework as the conventional oil and gas model. Specifically, the plan for updating estimates of the impact of ex situ oil shale and oil sands development in the Uinta Basin is to:

- 1. Estimate a range of possible future oil price paths based on EIA's Annual Energy Outlook oil price forecasts. This would involve converting EIA's AEO price forecasts into a probability distribution function from which we could randomly draw to come up with an arbitrary number of possible future oil price trends.
- 2. Rework their previous model for determining the break-even price of an oil shale or oil sands project (ISCE, 2013) to instead use Monte-Carlo methods for selecting important and/or uncertain model inputs (e.g. oil shale grade, thickness of oil sand deposit, labor requirements for processing equipment, etc.). With this methodology, a range of possible oil prices at which one might expect development to occur could be determined.
- 3. Randomly determine draws from both the oil price and oil shale/sands break-even price distributions. If in any given time step the oil price exceeds the break-even price, assume that a plant is built and track its impact on the region over time in the same areas discussed for conventional oil and gas (fiscal impacts, employment, water usage, air pollutants, etc.).

Subtask 3.4 - V/UQ Analysis of Basin Scale CLEARuff Assessment Tool (PI: Jennifer Spinti)

A summary of progress in this subtask is included with the Subtask 3.3 summary above.

Task 4.0 - Liquid Fuel Production by In-situ Thermal Processing of Oil Shale/Sands

Subtask 4.1 (Phase II) - Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil Shale/Sands (PI: Philip Smith)

The final deliverable for this project, a topical report detailing V/UQ studies on product yields as a function of operating conditions for indirectly heated rubblized oil shale beds, has a revised due date of March 2015. Researchers will continue to develop their HPC simulation tools for rubberized oil shale beds jointly with Subtask 7.3.

There are various strategies for simulating flow through a rubblized bed of oil shale. In the past, project researchers have concentrated on resolving each piece of oil shale as well as all channels among all of the rubblized pieces. However, this simulation approach requires enormous computational resources to resolve flow through the small convective channels (~ 1 mm) and to simulate heat transfer on the order of months for the entire bed. In the past quarter, project researchers have started to implement a new approach that simulates flow through porous media.

Flow through porous media incorporates a different set of physics than has been used previously in this project. The convective channels in the rubblized bed are represented by an overall solid porosity which defines the volume fraction of voids in a representative rubblized oil shale bed. Therefore, instead of explicitly resolving each channel, a property is used to represent all channels. Project researchers have begun incorporating this physics into an example geometry. However, the majority of their effort this quarter was spent on Subtask 7.3.

Subtask 4.2 - Reservoir Simulation of Reactive Transport Processes (PI: Milind Deo)

The research team is completing the final deliverable, a topical report on validation results for core-scale oil shale pyrolysis. They will be submitting the report during the next quarter.

Subtask 4.3 - Multiscale Thermal Processes (PI: Milind Deo, Eric Eddings)

There were no milestones or deliverables for this task due during the quarter. The research team has focused on generating additional TGA data at low pyrolysis rates and developing a mechanistic model of oil shale kerogen pyrolysis based on the CPD model.

Comparison of Oil Shale Pyrolysis Models

The research team continued its examination of pyrolysis rates at low heating rates that began in February, 2014. They re-calibrated the thermogravimetric analyzer (TGA) using magnets and curie point metals at heating rates of 0.5 and 1.0 K/min to ensure accurate temperatures. The new TGA data match previous BYU data at these heating rates (Hillier et al, 2010; Hillier and Fletcher, 2011). Data from the 0.5 and 1.0 K/min experiments were presented in the previous quarterly report. This quarter team members performed TGA experiments at heating rates of 0.25 K/min. These data were not repeatable due to noise and control problems associated with the long experimental times involved.

Chemical Percolation Devolatilization (CPD) Model

As knowledge of the characterization of shale oil increases due to modern solid-state Nuclear Magnetic Resonance (NMR), mass spectrometry, and gas chromatography, researchers are trying to improve the mechanistic description of oil shale pyrolysis. Current models empirically fit the mass released and may model individual species or tar. Mechanistic models may be able to describe oil shale pyrolysis over a broader range of heating conditions (heating rate, temperature, and pressure). The CPD model is a mechanistic pyrolysis model originally developed by Fletcher et al. (1989, 1992) to describe coal pyrolysis. Coal is modeled as a system of aromatic clusters connected by aliphatic bridges. During pyrolysis, aliphatic bridges are either (a) cleaved, leaving two side chains, or (b) transformed into a stable char bridge by releasing their aliphatic portion. A Bethe lattice is used to describe the parent chemical structure, with features such as cluster molecular weight, side chain molecular weight, and the number of attachments per cluster determined by solid-state ¹³C NMR measurements. Percolation lattice statistics are used to relate the temperature-dependent rate of aliphatic bridge breaking to the number of clusters that are detached from the original infinite lattice. Detached clusters form a liquid pool that can evaporate as tar, depending on the vapor pressure of each cluster. Tar is defined as any volatile matter that will later condense at room temperature. Detached clusters that remain too long with the solid will crosslink to the char. The CPD model has been used successfully to describe pyrolysis of a variety of fuels including coal and biomass (Fletcher et al., 1992; Fletcher et al., 2012; Lewis and Fletcher, 2013).

Since the chemical structure of oil shale was recently measured in detail using solid-state ¹³C NMR, the CPD model seemed like a logical choice for a mechanistic pyrolysis model. The kerogen structure parameters used in the CPD model are shown in Table 3 for the GR1.9, GR2.9, and GR3.9 samples, as reported by Solum et al. (2014).

	GR1.9	GR2.9	GR3.9
MW	776	775	946
MW	131	148	135
Attachments per cluster (σ +1)	5.0	4.5	5.9
Fraction of attachments that are bridges (p	0.5	0.5	0.5

Table 3. Chemical structure parameters measured for the GR1.9, GR2.9, and GR3.9 kerogen samples (Solum et al., 2014).

 $*p_0$ could not be measured by the NMR technique for oil shale, but was assumed to be 0.5.

The bridge-breaking scheme in the CPD model is shown in Figure 5. An aliphatic "labile" bridge (\pounds) is activated (\pounds^*) and is either cleaved to form two side chains (δ) with rate k_{δ} , or is transformed into a stable bridge (c) (such as a bi-aryl bridge) while releasing the aliphatic material (with rate k_c). The side chains will eventually degrade to form gases as well (with rate k_g). Experience has shown that the ratio of k_{δ}/k_c is relatively constant. The gas that is produced by the side chains that break off is referred to as g_1 whereas the gas that is produced by the bridge transformation to a char bridge is referred to as g_2 .



Figure 5. Bridge-breaking scheme used in the CPD model.

Predictions were made with the CPD model using the chemical structure parameters in Table 3 and the rate parameters for bridge breaking originally assigned for coal pyrolysis. These predictions did not compare well with the data obtained in the kerogen retort by Hillier et al. (2011) and by Fletcher et al. (2014). The next step was to use the rate coefficients determined for a first-order distributed activation energy model (DAEM) using TGA pyrolysis data reported in the October 2012 quarterly report. These rate coefficients (see Table 4) were used in the CPD model for both k_{δ} and k_c . In this table, each k is an Arrhenius rate constant, with pre-exponential factor A, mean activation energy E, and standard deviation in the activation energy σ . Activation energies are normalized by the universal gas constant R. Predicted and measured yields of char and tar using the rate coefficients from Table 4 are shown in Figure 6. It can be seen that the predicted tar yield (black line) is quite low, assuming that the tar consists only of material containing an aromatic cluster (which is a good assumption for coal). **Table 4.** Rate coefficients determined for a first-order DAEM model for the GR1, GR2, and GR3 oil shale samples from TGA data at three heating rates.

	A (s	E/R (K)	σ/R (K)
GR1	9.21 x 10	26,800	481
GR2	2.63 x 10	27,400	313
GR3	9.35 x 10	26,600	553



Figure 6. Initial CPD predictions of tar and char yields for GR3.9 kerogen pyrolysis at 10 K/min. Data are from Fletcher et al. (2014).

At first, the prediction of a low tar yield was quite puzzling. However, kerogen in oil shale has a carbon aromaticity of only 20% compared to 70-80% in coal (Solum et al., 2014; Fletcher et al., 2014; Solum et al., 1989; Boucher et al., 1991). The average molecular weight of a side chain in an unreacted coal ranges from 12 to 60 amu, whereas the side chain molecular weights in oil shale are 130-150 amu. The side chains in the oil shale kerogen are therefore 11 to 13 carbons in length, and the gases formed during pyrolysis of these side chains have a sufficiently large molecular weight to condense at room temperature and pressure. Therefore, if tar is defined as the volatile matter that condenses, a significant component of the tar will be the long chain aliphatic material that is not necessarily connected to an aromatic cluster. The carbon aromaticity of the tar from these samples was measured to be 19% (Solum et al., 2014).

A rough guess was made that 80% of the mass of released side chain material would be condensable and therefore counted as tar. The green line in Figure 6 shows a CPD model prediction with 80% of the "light" gas counted as tar in a post-processing step. This prediction shows reasonable agreement with the measured tar yield. The char yield was unaffected by the assignment of "light gas" as tar. The CPD model was changed to incorporate this 80% factor into the flash calculation, and the resulting predictions using the TGA rates for each kerogen sample are shown in Figure 7. The agreement is generally good, but the data indicate earlier release of light gas than predicted by the model.



Figure 7. CPD model calculations of tar and char yields for kerogen pyrolysis at 10 K/min using rate coefficients from Table 5 and counting 80% of the "light gas" as tar. Data are from Fletcher et al. (2014).

Researchers performed a literature search to see if there were any data to show that 80% of side chains in oil shale kerogen were of high enough molecular weight to condense at room temperature. The only data available are after pyrolysis. Therefore, the kerogen retort data from Fletcher et al. (2014) that show a tar yield are as good as any data available for determining this split. These data raise the question if there might be a difference in the two pathways for "light gas" formation shown earlier in Figure 5. Researchers arbitrarily assigned g_2 as light gas and g_1 as heavy gas in an attempt to remove the empiricism of assigning 80% of the light gas to be tar. The molecular weight of the light gas (MW_{lg}) was set to 20 amu and that of the heavy gas (MW_{hg}) was then calculated from the combined gas molecular weight (calculated from the NMR parameters by the CPD model), as follows:

$$y_{lg}MW_{lg} + y_{hg}MW_{hg} = MW_{all\ gases} \tag{1}$$

where $y_{lg} = g_2/(g_1 + g_2)$, $y_{hg} = g_1/(g_1 + g_2)$, and y_{lg} and y_{hg} were set to 0.2 and 0.8, respectively.

The reaction rate coefficients were then adjusted slightly to obtain the best fit with the kerogen retort data of Fletcher et al. (2014). The new rate coefficients are shown in Table 5, corresponding to the rate constants shown in Figure 5. Results of this prediction are shown in Figure 8. No empirical factor was used to count part of the light gas as tar, other than assigning g_1 as tar. This distinction between light gas and heavy gas allowed the model to predict the early light gases that came off before the tar. The fact that much of the light gas has already left the kerogen is apparent in the graph and show that it is necessary to have two different reaction constants. The overall agreement with this modeling approach with the CPD model is very good.

	GR1.9	GR2.9	GR3.9
A _{δ(}	9.8 x 10	9.8 x 10	1.8 x 10
Eδ	23,900	23,900	25,918
σεδ	0	0	0
Ag	1.58 x 10	2.58 x 10	1.58 x 10
Eg	21,000	21,000	27,600
σ_{Eg}	300	300	300
k _δ	0.9	0.9	1.8

Table 5. Rate coefficients determined for bridge breaking in the CPD model for the GR1.9, GR2.9, and GR3.9 kerogen samples to fit the kerogen retort data of Fletcher et al (2014).

In conclusion, it is apparent that much of what is classified as tar (i.e., condensables at room temperature) comes from aliphatic side chain material that is 11-13 carbons in length. The condensable aliphatic material seems to constitute about 80% of the total aliphatic material. Rate coefficients were modified in the CPD model to fit tar and char yields from kerogen retort experiments at 10 K/min. Model agreement was good if 80% of the aliphatic side chains were assigned as tar. However, this approach did not yield good agreement with the light gas release rate. In an effort to be more mechanistic, light gases were assumed to come only from char bridge formation and heavy gases were assumed to come only from aliphatic bridge cleavage. This assignment of light and heavy gases resulted in very good agreement with the kerogen retort data for the three kerogen samples studied.

In the next quarter, researchers plan to look more carefully at the capabilities of the CPD model approach to describe the changes in chemical structure during pyrolysis measured by Fletcher et al. (2014) and Hillier (2011) such as elemental composition of the char, carbon aromaticity, and length of side chains in the char.



Figure 8. CPD model calculations of tar and char yields for kerogen pyrolysis at 10 K/min using rate coefficients from Table 5 and assigning g_2 as the "light gas" and g_1 as the condensable "heavy gas". Data are from Fletcher et al. (2014).

Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions (PI: Milind Deo)

This project has been completed.

Subtask 4.5 - In Situ Pore Physics (PI: Jan Miller, Chen-Luh Lin)

This project has been completed.

Subtask 4.6 - Atomistic Modeling of Oil Shale Kerogens and Oil Sand Asphaltenes (PI: Julio Facelli)

This project has been completed.

Subtask 4.7 - Geomechanical Reservoir State (PI: John McLennan)

The milestone to complete the experimental matrix was completed in May 2014 and a short report was submitted to the program manager, Robert Vagnetti. The testing apparatus, which is a shared expenditure with other parties, was not available this quarter as had been previously anticipated. It has now been configured back to where oil shale testing can resume in the next quarter.

Subtask 4.8 - Developing a Predictive Geologic Model of the Green River Oil Shale, Uinta Basin (PI: Lauren Birgenheier)

The project team is planning to submit a book chapter that will replace the final report.

Subtask 4.9 - Experimental Characterization of Oil Shales and Kerogens (PI: Julio Facelli)

The paper entitled "Characterization of Macromolecular Structure Elements from a Green River Oil Shale, II. Characterization of Pyrolysis Products by ¹³C NMR, GC/MS, and FTIR," was finally published. The reference is included in the "Publications" section of this report.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

<u>Subtask 5.1 – Models for Addressing Cross-Jurisdictional Resource Management (PI: Robert Keiter, John Ruple)</u>

This project has been completed.

Subtask 5.2 - Conjunctive Management of Surface and Groundwater Resources (PI: Robert Keiter, John Ruple)

This project has been completed.

<u>Subtask 5.3 - Policy and Economic Issues Associated with Using Simulation to Assess</u> <u>Environmental Impacts (PI: Robert Keiter, Kirsten Uchitel)</u>

No report received. A final report on this project is due.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

Subtask 6.1 Engineering Process Models for Economic Impact Analysis (PI: Terry Ring)

This project has been completed.

Subtask 6.2 - Policy analysis of the Canadian oil sands experience (PI: Kirsten Uchitel)

This project has been completed

Subtask 6.3 - Market Assessment Report (PI: Jennifer Spinti)

This project has been completed

7.0 – Strategic Alliance Reserve

Subtask 7.1 – Geomechanical Model (PI: John McLennan)

During this quarter, the project team continued to move forward on several fronts. Segmented linearization and development of constitutive modeling surfaces is proceeding using an undergraduate working with a Ph.D. candidate. Simulations of the triaxial testing are being carried out using FLAC3D as described below. Team members continue to debug the relative permeability apparatus that they will be using to infer oil shale permeability before and after pyrolysis. Finally, they have been developing reservoir scale simulations (also using FLAC3D) to simulate the entire reservoir development process, including heating, porosity and permeability development and associated stress and deformation changes.

In the next quarter, the project team plans to perform additional triaxial testing. This will be designed to simulate the actual heating process. The stresses (or boundary deformation) will be maintained constant and heating applied to provide a realistic representation of how an element of oil shale will deform. Both the completed and planned triaxial testing will be simulated using FLAC3D. Lastly, absolute permeability measurements will be carried out, and reservoir scale simulations of subsidence will continue.

Numerical Simulation of Triaxial Testing

The project team has initially used data provided by AMSO to develop protocols for performing the simulations. Some basic programming has been involved to increase the capabilities of the commercial codes. Many trials have been run in the last two months using FLAC3D®. This code is adaptable for simulating a layered, continuous medium which is subjected to increasing deviatoric stress (as is applied in a conventional triaxial test), hydrostatic confining pressure (representing in-situ horizontal stresses), and increasing temperature.

Team members have been applying confining pressure and deviatoric stress to cylindrical surrogate samples in order to duplicate laboratory measurements; deviatoric stress is increased with time. The effect of temperature on the properties and behavior of the oil shale will be considered later after satisfactory representation of axial and radial deformation under increasing deviatoric stress (stress applied axially to the sample).

Figures 9 and 10 illustrate recent results. Figure 9 shows displacement of an oil shale sample as axial load was increasingly applied from the top. The two undeformed sections at the top and bottom are stainless steel end caps. The middle of the oil shale deformed radially; the axial sample deformed linearly at first followed by hyperbolic behavior. Phase conversion (conversion of solid kerogen to gas or liquids), while not yet explicitly considered, is implicitly represented by increased deformability.



Figure 9. This illustration shows the deformation of a cylindrical oil shale sample subjected to increasing temperature. Issues being investigated include whether or not surface subsidence will occur as a result of vertical deformation of oil shale zones as a result of pyrolysis.

Figure 10 represents the curve of total load (deviatoric stress and confining stress multiplied by the cross sectional area of the sample) applied to the top end cap. Because of sign conventions used in the software, increasing compressional load and deformation have negative signs and the axial deformation and load increase to the left and down respectively. The early time fluctuations are numerical artifacts that are being rectified.



Figure 10. Axial deformation (tension positive, x-axis) versus axial load (tension positive, y-axis) showing progressively accelerated deformation at relatively low stress levels.

Subtask 7.2 - Kinetic Compositional Models and Thermal Reservoir Simulators (PI: Milind Deo)

Project has been terminated.

Subtask 7.3 – Rubblized Bed High Performance Computing Simulations (PI: Philip Smith)

In this quarter, researchers have continued their development of High Performance Computing (HPC) simulation tools for in-situ thermal treatment of oil shale. They have moved away from the AMSO process and started to perform simulations of oil shale retorting as it may be realized during a commercial phase. These simulations include kinetic compositional models which would estimate the oil yield for this scenario. However, because of the computational demands, the formation has not been sufficiently heated to produce any oil. Therefore, the milestone of performing a generation 2 simulation with kinetic compositional models incorporated is still in progress and will be completed in the next quarter.

From the onset of this capstone project, researchers have concentrated their efforts on simulating heater experiments conducted by AMSO at their pilot test facility in Rifle, CO. In the first quarter of 2014, they completed simulations of both AMSO heater tests using the co-simulation strategy introduced previously. These results were presented at the STAR Global Conference in March 2014 and summarized in the April 2014 quarterly report. Also, at the end of April, team members met with AMSO scientists at the University of Utah to review the final results.

After the successful completion of simulations of the AMSO heater tests, team members have focused on simulations that would capture a domain which is much closer to a commercial scale employed for in-situ oil shale retorting. Such a domain is shown in Figure 11. This 0.25 km x 0.25 km x 0.25 km domain captures five heating wells, for which the horizontal heating section is 100 meters long. It is assumed that the vertical and curved section of each well is insulated from the heating fluid circulating in the hot horizontal section.



Figure 11. Extended domain used in current generation of simulations of in-situ thermal retorting of oil shale.

For this simulation, researchers have included the detailed property variations as a function of depth and temperature. This property variation can be seen in Figure 12 in the vertical plane, which also shows the mesh refinement in the domain. The mesh is very fine (~ 1 cm) near the well and is gradually coarsened away from the well, resulting in approximately 300 million cells in the computational domain.



Figure 12. Extended domain simulation with mesh on the vertical plane and temperature distribution in the horizontal plane. The scale bar relates to the temperature distribution.

CONCLUSIONS

Significant research progress was made in all the research programs that have yet to be completed. Researchers in Subtasks 4.1 and 7.3, who are using HPC tools to simulated in situ oil shale processes, have moved to larger scales that are more representative of commercial-scale facilities. In related research, team members in Subtasks 4.8 and 7.1 made progress on reservoir scale simulations that include large scale deformation with the application of high temperature. Data for these simulations is being collected in a triaxial testing device developed by ISCE researchers. The Subtask 4.3 team is developing a mechanistic model of oil shale kerogen pyrolysis based on the CPD model. Finally, a skeletal model of oil and gas development in the Uinta Basin has been completed. This model will be coupled to previous work on oil shale/sands development to create a tool for estimating what future development scenarios might look like.

COST PLAN/STATUS

	Yr. 1							Yr. 2				
Receipe Reporting Quarter BHASE I	Q1		Q	2		Q3	C	14	Q5		Q6	
Baseline Reporting Quarter - FRASE I	7/1/09 - 1	2/31/09	1/1/10 -	3/31/10	4/1/10	- 6/30/10	7/1/10 -	9/30/10	10/1/10 -	12/31/10	1/1/11 - 3/31/11	
	Q1	Total	Q2	Total	Q3	Total	Q4	Total	Q5	Total	Q6	Total
Baseline Cost Plan												
Federal Share	484,728	484,728	484,728	969,456	484,728	1,454,184	484,726	1,938,910	323,403	2,262,313	798,328	3,060,641
Non-Federal Share	121,252	121,252	121,252	242,504	121,252	363,756	121,254	485,010	80,835	565,845	199,564	765,409
Total Planned	605,980	605,980	605,980	1,211,960	605,980	1,817,940	605,980	2,423,920	404,238	2,828,158	997,892	3,826,050
Actual Incurred Cost												
Federal Share	420,153	420,153	331,481	751,634	547,545	1,299,179	428,937	1,728,116	593,386	2,321,502	307,768	2,629,270
Non-Federal Share	29,456	29,456	131,875	161,332	151,972	313,304	100,629	413,933	191,601	605,534	45,101	650,635
Total Incurred Costs	449,609	449,609	463,356	912,966	699,517	1,612,483	529,566	2,142,049	784,987	2,927,036	352,869	3,279,905
Variance												
Federal Share	64,575	64,575	153,247	217,822	-62,817	155,005	55,789	210,794	-269,983	-59,189	490,560	431,371
Non-Federal Share	91,796	91,796	-10,623	81,172	-30,720	50,452	20,625	71,077	-110,766	-39,689	154,463	114,774
Total Variance	156,371	156,371	142,624	298,994	-93,537	205,457	76,414	281,871	-380,749	-98,878	645,023	546,145

Note: Q5 and Q6 reflect both CDP 2009 and CDP 2010 SF424a projections as the award periods overlap.

	Yr. 2			Yr. 3								
Desire Desire Oracle Division	Q	7	Q8		Q9		Q10		Q11		Q12	
Baseline Reporting Quarter - PHASE II	04/01/11 -	06/30/11	07/01/11 -	09/30/11	10/01/11	- 12/31/11	01/1/12 -	03/31/12	04/01/12	- 06/30/12	07/01/12 -	09/30/12
	Q7	Total	Q8	Total	Q9	Total	Q10	Total	Q11	Total	Q12	Total
Baseline Cost Plan												
Federal Share	712,385	3,773,026	627,423	4,400,449	147,451	4,547,900	147,451	4,695,351	147,451	4,842,802	245,447	5,088,249
Non-Federal Share	178,100	943,509	156,854	1,100,363	36,863	1,137,226	36,863	1,174,089	36,863	1,210,952	58,906	1,269,858
Total Planned	890,485	4,716,535	784,277	5,500,812	184,314	5,685,126	184,314	5,869,440	184,314	6,053,754	304,353	6,358,107
Actual Incurred Cost												
Federal Share	449,459	3,078,729	314,813	3,393,542	271,897	3,665,439	267,784	3,933,223	191,438	4,124,661	232,367	4,357,028
Non-Federal Share	48,902	699,537	48,835	748,372	105,695	854,067	40,652	894,719	33,092	927,811	44,294	972,105
Total Incurred Costs	498,361	3,778,266	363,648	4,141,914	377,592	4,519,506	308,436	4,827,942	224,530	5,052,472	276,661	5,329,133
Variance												
Federal Share	262,926	694,297	312,610	1,006,907	-124,446	882,461	-120,333	762,128	-43,987	718,141	13,080	731,221
Non-Federal Share	129,198	243,972	108,019	351,991	-68,832	283,159	-3,789	279,370	3,771	283,141	14,612	297,753
Total Variance	392,124	938,269	420,629	1,358,898	-193,278	1,165,620	-124,122	1,041,498	-40,216	1,001,282	27,692	1,028,974

	Yr. 4								Yr. 5			
Pasalina Reporting Quarter BHASE II	Q1	3	Q	14	C	215	Q16 - R	EVISED	Q	17	Q18	
Baseline Reporting Quarter - PHASE II	10/01/12 -	12/31/12	01/01/13 -	03/31/13	04/01/13	- 06/30/13	07/01/13	- 09/30/13	10/01/13	- 12/31/13	01/01/14 -	03/31/14
	Q13	Total	Q14	Total	Q15	Total	Q16	Total	Q17	Total	Q18	Total
Baseline Cost Plan												
Federal Share	146,824	5,235,073	146,824	5,381,897	146,824	5,528,721	-471,238	5,057,483	157,250	5,214,733	157,250	5,371,983
Non-Federal Share	36,705	1,306,563	36,705	1,343,268	36,705	1,379,973	-211,982	1,167,991	53,484	1,221,475	53,484	1,274,959
Total Planned	183,529	6,541,636	183,529	6,725,165	183,529	6,908,694	-683,220	6,225,474	210,734	6,436,208	210,734	6,646,942
Actual Incurred Cost												
Federal Share	128,349	4,485,377	180,613	4,665,990	233,732	4,899,722	157,761	5,057,483	113,187	5,170,670	148,251	5,318,921
Non-Federal Share	79,871	1,051,976	62,354	1,114,330	51,708	1,166,038	1,953	1,167,991	66,131	1,234,122	48,378	1,282,500
Total Incurred Costs	208,220	5,537,353	242,967	5,780,320	285,440	6,065,760	159,714	6,225,474	179,318	6,404,792	196,629	6,601,421
Variance												
Federal Share	18,475	749,696	-33,789	715,907	-86,908	628,999	-628,999	0	44,063	44,063	8,999	53,062
Non-Federal Share	-43,166	254,587	-25,649	228,938	-15,003	213,935	-213,935	0	-12,647	-12,647	5,106	-7,541
Total Variance	-24,691	1,004,283	-59,438	944,845	-101,911	842,934	-842,934	0	31,416	31,416	14,105	45,521

Note: Baseline Cost Plan adjusted in Q16 to reflect NCE projections.

	Yr. 5							
Baseline Reporting Quarter - PHASE II	Q1	9	Q20					
	04/01/14 -	06/30/14	07/01/14	- 09/30/14				
	Q19	Total	Q20	Total				
Baseline Cost Plan								
Federal Share	157,250	5,529,233	133,282	5,662,515				
Non-Federal Share	53,484	1,328,443	87,436	1,415,879				
Total Planned	210,734	6,857,676	220,718	7,078,394				
Actual Incurred Cost								
Federal Share	147,582	5,466,503		5,466,503				
Non-Federal Share	46,472	1,328,971		1,328,971				
Total Incurred Costs	194,053	6,795,474	0	6,795,474				
Variance								
Federal Share	9,668	62,730	133,282	196,012				
Non-Federal Share	7,012	-528	87,436	86,908				
Total Variance	16,681	62,202	220,718	282,920				

MILESTONE STATUS

п	Title/Description	Planned Completion	Actual Completion	Milestone
1.0	Project Management	Date	Date	Otatus
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-13	N/A	Decision has been made to disband EAB
	Hold final project review meeting	Jun-13		this meeting until
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in CLEAR CO2 emissions from conventional oil & gas development in the Uinta Basin	Nov-14		Milestone date has been changed to reflect new project timelines
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Sep-12	Oct-12	Report attached as appendix to Oct. 2012 quarterly report
3.3	Development of oil & gas production modules for CLEAR			
	Develop preliminary modules in CLEAR for conventional oil & gas development & produced water management in Uinta Basin	Oct-11	Dec-11	Discussed in Jan. 2012 quarterly report
3.4	V/UQ analysis of basin scale CLEAR assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11	Nov-11	Discussed in Jan. 2012 quarterly report
	Demonstrate full functionality of V/UQ methodology for conventional oil development in Uinta Basin	Nov-13	Apr-14	Demonstration delayed until first quarter of 2014
	Demonstrate full functionality for conventional & unconventional oil development in Uinta Basin	Mar-14	Jun-14	Discussed in this quarterly report
4.0	Liquid Fuel Production by In-Situ Thermal Processing of Oil Shale/Sands			
4.1	Development of CFD-based simulation tool for in-situ thermal processing of oil shale/ sands			

п	Title/Description	Planned Completion	Actual Completion	Milestone
שו	Expand modeling to include reaction	Date	Date	
	chemistry & study product yield as a function of operating conditions	Feb-12	Mar-12	Discussed in April 2012 quarterly report
4.2	Reservoir simulation of reactive transport processes			
	Incorporate kinetic & composition models into both commercial & new reactive transport models	Dec-11	Dec-11	Discussed in Jan. & July 2012 quarterly reports
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12	Jun-12	Discussed in July 2012 quarterly report
4.3	Multiscale thermal processes			
	Complete thermogravimetric analyses experiments of oil shale utilizing fresh "standard" core	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete core sample pyrolysis at various pressures & analyze product bulk properties & composition	Dec-11	Sep-12	Discussed in Oct. 2012 quarterly report
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12	Jun-12	Discussed in July 2012 quarterly report
4.5	In situ pore physics			
	Complete pore network structures & permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various loading conditions, pyrolysis temperatures, & heating rates	Mar-12	Mar-12	Discussed in April 2012 quarterly report; PI dropped loading condition as variable
4.6	Atomistic modeling of oil shale kerogens & oil sand asphaltenes			
	Complete web-based repository of 3D models of Uinta Basin kerogens, asphaltenes, & complete systems (organic & inorganic materials)	Dec-11	Dec-11	Discussed in Jan. 2012 quarterly report
4.7	Geomechanical reservoir state			
	Complete high-pressure, high-temperature vessel & ancillary flow system design & fabrication	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete experimental matrix	Mar-14	May-14	Report sent to R. Vagnetti on 27 May 2014
	Complete thermophysical & geomechanical property data analysis & validation	Dec-14		Due date has been revised to reflect status of expts.

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin			
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
	Detailed mineralogic & geochemical analysis of same cores	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Feb-12	Email sent to R. Vagnetti on Feb. 6, 2012 & discussed in April 2012 quarterly report
	Development of a structural model of kerogen & bitumen	Jun-12	Jun-12	Discussed in July 2012 quarterly report
5	Environmental, legal, economic, & policy framework			
5.1	Models for addressing cross-jurisdictional resource management			
	Identify case studies for assessment of multi-jurisdictional resource management models & evaluation of utility of models in context of oil shale & sands development	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
5.2	Conjunctive management of surface & groundwater resources			
	Complete research on conjunctive surface water & groundwater management in Utah, gaps in its regulation, & lessons that can be learned from existing conjunctive water management programs in other states	Aug-11	Aug-11	Discussed in Oct. 2011 quarterly report
5.3	Policy & economic issues associated with using simulation to assess environmental impacts			
	White paper describing existing judicial & agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis	Dec-12	Dec-12	Submitted with Jan. 2103 quarterly report
6	Economic & policy assessment of domestic unconventional fuels industry			
6.1	Engineering process models for economic impact analysis			
	Upload all models used & data collected to repository	Oct-12	Aug-13	All models/data have been uploaded to the ICSE website

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
7	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
7.1	Geomechanical model			
	Make experimental recommendations	Aug-13	Aug-13	Discussed in this quarterly report
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Dec-14		Due date has been revised to reflect status of expts.
	Basic reservoir simulations to account for thermal front propagation	Mar-15		Due date has been revised to reflect status of expts.
	Evaluation of flow mechanics	Mar-15		Due date has been revised to reflect status of expts.
7.2	Kinetic compositional models & thermal reservoir simulators			Project has been terminated
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12	Jun-12	Discussed in July 2012 quarterly report
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12	Jun-12	Discussed in July 2102 quarterly report
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Sep-14		Delayed due to priorities of AMSO

NOTEWORTHY ACCOMPLISHMENTS

Nothing to report.

PROBLEMS OR DELAYS

Several milestone due dates have been revised to reflect the status of the research. These changes are reflected in the "Milestone Status" chart above.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

- Spinti, J. (2013, January 10). Presenter/panelist *The real impact of oil shale and oil sands development in Utah.* 2013 Governor's Energy Development Summit, Salt Lake City, UT.
- Hradisky, M., Smith, P. J. & Burnham, A. (2013, March). *STAR-CCM+ simulations of in-situ thermal treatment of oil shale*. Paper presented at the STAR Global Conference, Orlando, FL, March 18-20, 2013.
- Orendt, A. M., Solum, M. S., Facelli, J. C., Pugmire, R. J., Chapman, K. W., Winans, R. E. & Chupas, P. (2013, April). Characterization of shale and kerogen from a Green River oil shale core, ENFL-535. Paper presented at the 245th American Chemical Society National Meeting, New Orleans, LA, April 7-11, 2013.
- Birgenheier, L. P. (2013, May 7). Presenter/panelist *Constructing a basin-wide geologic model*. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Smith, P. J. (2013, May 7). Presenter/panelist *Simulation of in situ production process using computational fluid dynamics*. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Spinti, J. P. (2013, May 7). Presenter/panelist Assessment of unconventional fuels development costs. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Birgenheier, L.P., Plink-Bjorklund, P., Vanden Berg, M.D., Rosenberg, M., Toms, L. & Golab, J. (2013). A genetic stratigraphic framework of the Green River Formation, Uinta Basin, Utah: The impact of climatic controls on lake evolution. Paper presented at the American Association of Petroleum Geologists Annual Meeting, Pittsburgh, PA, May 22-25, 2013.
- Vanden Berg, M. D., Eby, D. E., Chidsey, T. C. & Laine, M.D. (2013). *Microbial carbonates in cores from the Tertiary (Eocene) Green River Formation, Uinta Basin, Utah, U.S.A.: Analogues for non-marine microbialite oil reservoirs worldwide*. Paper presented at Microbial Carbonates in Space and Time: Implications for Global Exploration and Production, The Geological Society, London, United Kingdom, June 19-20, 2013.
- Rosenberg, M. J. (2013). Facies, stratigraphic architecture, and lake evolution of the oil shale bearing Green River Formations, eastern Uinta Basin, Utah. M.S. thesis, Department of Geology and Geophysics, University of Utah.
- Tiwari, P., Deo, M., Lin, C. L. & Miller, J.D. (2013, May). Characterization of oil shale pore structure before and after pyrolysis by using X-ray micro CT. *Fuel*, *107*, 547–554.

- Pugmire, R. J., Fletcher, T. H., Hillier, J., Solum, M., Mayne, C. & Orendt, A. (2013, October). Detailed characterization and pyrolysis of shale, kerogen, kerogen chars, bitumen, and light gases from a Green River oil shale core. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M.S. & Pugmire, R. J. (2013, October). Characterization of pyrolysis products from a Utah Green River oil shale by ¹³C NMR, GC/MS, and FTIR. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Wilkey, J., Spinti, J., Ring, T., Hogue, M. & Kelly, K. (2013, October). Economic assessment of oil shale development scenarios in the Uinta Basin. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Hillier, J. L., Fletcher, T. H., Solum, M. S. & Pugmire, R. J. (2013, October). Characterization of macromolecular structure of pyrolysis products from a Colorado Green River oil shale. Accepted, *Industrial and Engineering Chemistry Research*. dx.doi.org/10.1021/ie402070s
- Birgenheier, L. & Vanden Berg, M. (n.d.). Facies, stratigraphic architecture, and lake evolution of the oil shale bearing Green River Formation, eastern Uinta Basin, Utah. To be published in Smith, M. and Gierlowski-Kordesch, E. (Eds.). *Stratigraphy and limnogeology of the Eocene Green River Formation*, Springer.
- Solum, M. S., Mayne, C. L., Orendt, A. M., Pugmire, R. J., Hall, T., Fletcher, T. H. (2014). Characterization of macromolecular structure elements from a Green River oil shale-(I. Extracts). Submitted to *Energy and Fuels, 28*, 453-465. dx.doi.org/10.1021/ef401918u,
- Kelly, K.E., Wilkey, J. E. Spinti, J. P., Ring, T. A. & Pershing, D. W. (2014, March). Oxyfiring with CO₂ capture to meet low-carbon fuel standards for unconventional fuels from Utah. *International Journal of Greenhouse Gas Control, 22,* 189–199.
- Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M.S., and Pugmire, R. J. (2013, January). Characterization of macromolecular structure elements from a Green River oil shale, II. Characterization of pyrolysis products from a Utah Green River oil shale by ¹³C NMR, GC/MS, and FTIR. *Energy and Fuels, 28*, 2959-2970. dx.doi.org/10.1021/ef500095j
- Hradisky, M., Smith, P. J., Burnham, A. K. (2014, March). STAR-CCM+ high performance computing simulations of oil shale retorting system using co-simulation. Presented at the STAR Global Conference, Vienna, Austria. March 2014.
- Barfuss, D. C., Fletcher, T. H. Fletcher and Pugmire, R. J. (2014, October). Modeling oil shale pyrolysis using the Chemical Percolation Devolatilization model. Abstract submitted for a presentation at the 35th Oil Shale Symposium, Golden, CO, October 13-15, 2014.
- Hardisky, M. and Smith, P. J. (2014, October). Evaluation of well spacing and arrangement for in-situ thermal treatment of oil shale using HPC simulation tools. Abstract submitted for a presentation at the 35th Oil Shale Symposium, Golden, CO, October 13-15, 2014.

REFERENCES

Boucher, R. J., Standen, G. and Eglinton, G. (1991). Molecular characterization of kerogens by mild selective chemical degradation -- Ruthenium tetroxide oxidation. *Fuel*, *70(6)*, 695-702.

- Coraggio, G. & Laiola, M. (2009). Combustion of NG and pulverized coal in a mixture of oxygen and RFG (IFRF. Doc. No F110/y/01). Pisa, Italy: International Flame Research Foundation.
- Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M. S. and Pugmire, R. J. (2014). Characterization of macromolecular structure elements from a Green River oil shale, II. Characterization of pyrolysis products by ¹³C NMR, GC/MS, and FTIR. *Energy and Fuels*, 28, 2959-2970.
- Fletcher, T. H., Grant, D. M., Pugmire, R. J. and Kerstein, A. R. (1989). Chemical model of coal devolatilization using percolation lattice statistics. *Energy & Fuels*, *3*(*2*), 175-186.
- Fletcher, T. H., Kerstein, A. R., Pugmire, R. J., Solum, M. S. and Grant, D. M. (1992). Chemical percolation model for devolatilization. 3. Direct use of 13C NMR data to predict effects of coal type. *Energy & Fuels, 6(4)*, 414-431.
- Fletcher, T. H., Pond, H. R., Webster, J. and Baxter, L. L. (2012). Prediction of tar and light gas during pyrolysis of black liquor and biomass. *Energy and Fuels, 26*, 3381-3387.
- Institute for Clean and Secure Energy, (2013). A market assessment of oil shale and oil sands development scenarios in Utah's Uinta Basin. Salt Lake City, UT: The University of Utah.
- Hillier, J. L. (2011). Pyrolysis kinetics and chemical structure considerations of a Green River oil shale and its derivatives. Ph.D. dissertation, Chemical Engineering Department, Brigham Young University, Provo, UT.
- Hillier, J., Bezzant, T., Fletcher, T. H. (2010). Improved method for the determination of kinetic parameters from non-isothermal thermogravimetric analysis (TGA) data. *Energy & Fuels*, 24(5), 2841-2847.
- Hillier, J. L. and Fletcher, T. H. (2011). Pyrolysis kinetics of a Green River oil shale using a pressurized TGA. *Energy & Fuels, 25*, 232-239.
- Lewis, A. D. and Fletcher, T. H. (2013). Prediction of sawdust pyrolysis yields from a flat-flame burner using the CPD model. *Energy & Fuels*, *27*, 942-953.
- Solum, M. S., Mayne, C. L., Orendt, A. M., Pugmire, R. J., Hall, T. and Fletcher, T. H. (2014). Characterization of macromolecular structure elements from a Green River oil shale, I. Extracts. *Energy and Fuels, 28*, 453-465.
- Solum, M. S., Pugmire, R. J. and Grant, D. M. (1989). Carbon-13 solid-state NMR of Argonne premium coals. *Energy & Fuels, 3(2)*, 187-193.

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